CPSC 330 Applied Machine Learning

Lecture 5: Preprocessing and sklearn pipelines

UBC 2022-23

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Imports

```
In [1]:
            import sys
            import time
         3
            import matplotlib.pyplot as plt
         5
         6 %matplotlib inline
         7 import numpy as np
         8 import pandas as pd
            from IPython.display import HTML
        10
           sys.path.append("../code/.")
        11
        12
        13 import mglearn
            from IPython.display import display
        15 from plotting functions import *
        16
        17
           # Classifiers and regressors
        18 from sklearn.dummy import DummyClassifier, DummyRegressor
        19
        20 # Preprocessing and pipeline
        21 from sklearn.impute import SimpleImputer
        22
        23 # train test split and cross validation
        24 from sklearn.model selection import cross val score, cross validate, tr
        25 from sklearn.neighbors import KNeighborsClassifier, KNeighborsRegressor
            from sklearn.pipeline import Pipeline
           from sklearn.preprocessing import (
        27
        28
                MinMaxScaler,
        29
                OneHotEncoder,
        30
                OrdinalEncoder,
        31
                StandardScaler,
        32 )
        33 from sklearn.svm import SVC
        34 from sklearn.tree import DecisionTreeClassifier
        35 from utils import *
        36
        37 | pd.set_option("display.max colwidth", 200)
```

Announcements

- Homework 3 is out (Due date: Feb. 1st). Please start early.!
- Homework 1 grades and solutions are out. Please do not share them with anyone or do not post them anywhere.

Learning outcomes

From this lecture, you will be able to

- · explain the motivation for preprocessing in supervised machine learning;
- identify when to implement feature transformations such as imputation, scaling, and one-hot encoding in a machine learning model development pipeline;
- use sklearn transformers for applying feature transformations on your dataset;
- discuss the golden rule (a.k.a. don't look at the test set until the end) in the context of feature transformations;
- use sklearn.pipeline.Pipeline and sklearn.pipeline.make_pipeline to build a preliminary machine learning pipeline.

Motivation and big picture [video (https://youtu.be/xx9HlmzORRk)]

- · So far we have seen
 - Three ML models (decision trees, *k*-NNs, SVMs with RBF kernel)
 - ML fundamentals (train-validation-test split, cross-validation, the fundamental tradeoff, the golden rule)
- Are we ready to do machine learning on real-world datasets?
 - Very often real-world datasets need preprocessing before we use them to build ML models.

Example: k-nearest neighbours on the Spotify dataset

- In lab1 you used DecisionTreeClassifier to predict whether the user would like a
 particular song or not.
- Can we use a *k*-NN classifier for this task?
- Intuition: To predict whether the user likes a particular song or not (query point)
 - find the songs that are closest to the query point
 - let them vote on the target
 - take the majority vote as the target for the query point

Mean validation score 0.508

Out[3]:

	fit_time	score_time	test_score	train_score
0	0.004357	0.001195	0.507740	0.507752
1	0.000990	0.000347	0.507740	0.507752
2	0.000742	0.000344	0.507740	0.507752
3	0.000674	0.000306	0.506211	0.508133
4	0.000642	0.000300	0.509317	0.507359

```
In [4]:
```

```
1 knn = KNeighborsClassifier()
```

- 2 scores = cross_validate(knn, X_train, y_train, return_train_score=True)
 2 print("Moon_validation_ggore_%0.2f" % (nn_moon(ggoregg"togt_ggore"1)))
- 3 print("Mean validation score %0.3f" % (np.mean(scores["test_score"])))
- 4 pd.DataFrame(scores)

Mean validation score 0.546

Out[4]:

	fit_time	score_time	test_score	train_score
0	0.013952	0.018358	0.563467	0.717829
1	0.002404	0.009834	0.535604	0.721705
2	0.002058	0.008475	0.529412	0.708527
3	0.002010	0.008687	0.537267	0.721921
4	0.001937	0.008455	0.562112	0.711077

```
In [5]:
```

```
two_songs = X_train.sample(2, random_state=42)
two songs
```

Out[5]:

	acousticness	danceability	duration_ms	energy	instrumentalness	key	liveness	loudness	mo
842	0.229000	0.494	147893	0.666	0.000057	9	0.0469	-9.743	
654	0.000289	0.771	227143	0.949	0.602000	8	0.5950	-4.712	

```
In [6]: 1 euclidean_distances(two_songs)
```

```
Out[6]: array([[ 0. , 79250.00543825], [79250.00543825, 0. ]])
```

Let's consider only two features: duration ms and tempo.

```
two_songs_subset = two_songs[["duration_ms", "tempo"]]
In [7]:
             two songs subset
Out[7]:
             duration_ms
                        tempo
         842
                 147893 140.832
         654
                 227143 111.959
In [8]:
             euclidean_distances(two_songs_subset)
Out[8]: array([[
                                 , 79250.00525962],
                      0.
                [79250.00525962,
                                       0.
                                                  11)
```

Do you see any problem?

- · The distance is completely dominated by the the features with larger values
- The features with smaller values are being ignored.
- · Does it matter?
 - Yes! Scale is based on how data was collected.
 - Features on a smaller scale can be highly informative and there is no good reason to ignore them.
 - We want our model to be robust and not sensitive to the scale.
- Was this a problem for decision trees?

Scaling using scikit-learn's <u>StandardScaler (https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.StandardScaler</u>

- We'll use scikit-learn's <u>StandardScaler (https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.StandardScaler.html</u>), which is a transformer.
- Only focus on the syntax for now. We'll talk about scaling in a bit.

Out[9]:

	acousticness	danceability	duration_ms	energy	instrumentalness	key	liveness	loudn
0	-0.697633	-0.194548	-0.398940	-0.318116	-0.492359	1.275623	-0.737898	0.395
1	-0.276291	0.295726	-0.374443	-0.795552	0.598355	-1.487342	-0.438792	-0.052
2	-0.599540	1.110806	-0.376205	-0.946819	-0.492917	0.446734	-0.399607	-0.879
3	-0.307150	1.809445	-0.654016	-1.722063	-0.492168	0.170437	-0.763368	-1.460
4	-0.634642	0.491835	-0.131344	1.057468	2.723273	0.170437	-0.458384	-0.175

fit and transform paradigm for transformers

- sklearn uses fit and transform paradigms for feature transformations.
- We fit the transformer on the train split and then transform the train split as well as the test split.
- · We apply the same transformations on the test split.

sklearn API summary: estimators

Suppose model is a classification or regression model.

```
model.fit(X_train, y_train)
X_train_predictions = model.predict(X_train)
X_test_predictions = model.predict(X_test)
```

sklearn API summary: transformers

Suppose transformer is a transformer used to change the input representation, for example, to tackle missing values or to scales numeric features.

```
transformer.fit(X_train, [y_train])
X_train_transformed = transformer.transform(X_train)
X_test_transformed = transformer.transform(X_test)
```

- You can pass y_train in fit but it's usually ignored. It allows you to pass it just to be consistent with usual usage of sklearn's fit method.
- You can also carry out fitting and transforming in one call using fit_transform. But be mindful to use it only on the train split and **not** on the test split.
- Do you expect DummyClassifier results to change after scaling the data?
- Let's check whether scaling makes any difference for k-NNs.

```
In [10]: 1 knn_unscaled = KNeighborsClassifier()
2 knn_unscaled.fit(X_train, y_train)
3 print("Train score: %0.3f" % (knn_unscaled.score(X_train, y_train)))
4 print("Test score: %0.3f" % (knn_unscaled.score(X_test, y_test)))

Train score: 0.726
Test score: 0.552

In [11]: 1 knn_scaled = KNeighborsClassifier()
2 knn_scaled.fit(X_train_scaled, y_train)
3 print("Train score: %0.3f" % (knn_scaled.score(X_train_scaled, y_train))
4 print("Test score: %0.3f" % (knn_scaled.score(X_test_scaled, y_test)))

Train score: 0.798
Test score: 0.686
```

- The scores with scaled data are better compared to the unscaled data in case of k-NNs.
- I am not carrying out cross-validation here for a reason that we'll look into soon.
- Note that I am a bit sloppy here and using the test set several times for teaching purposes. But when you build an ML pipeline, please do assessment on the test set only once.

Common preprocessing techniques

Some commonly performed feature transformation include:

- Imputation: Tackling missing values
- Scaling: Scaling of numeric features
- One-hot encoding: Tackling categorical variables

We could have one lecture on each of them! In this lesson our goal is to getting familiar with them so that we can use them to build ML pipelines.

In the next part of this lecture, we'll build an ML pipeline using <u>California housing prices regression</u> <u>dataset (https://www.kaggle.com/harrywang/housing)</u>. In the process, we will talk about different feature transformations and how can we apply them so that we do not violate the golden rule.

Imputation and scaling [video (https://youtu.be/G2IXbVzKlt8)]

Dataset, splitting, and baseline

We'll be working on <u>California housing prices regression dataset</u> (https://www.kaggle.com/harrywang/housing) to demonstrate these feature transformation techniques. The task is to predict median house values in Californian districts, given a number of features from these districts. If you are running the notebook on your own, you'll have to download the data and put it in the data directory.

Out[12]:

	longitude	latitude	housing_median_age	total_rooms	total_bedrooms	population	households
6051	-117.75	34.04	22.0	2948.0	636.0	2600.0	602.0
20113	-119.57	37.94	17.0	346.0	130.0	51.0	20.0
14289	-117.13	32.74	46.0	3355.0	768.0	1457.0	708.0
13665	-117.31	34.02	18.0	1634.0	274.0	899.0	285.(
14471	-117.23	32.88	18.0	5566.0	1465.0	6303.0	1458.0

Some column values are mean/median but some are not.

Let's add some new features to the dataset which could help predicting the target: median house value.

```
train_df = train_df.assign(
In [13]:
           1
                 rooms per household=train df["total rooms"] / train df["households"
           2
           3
           4
             test_df = test_df.assign(
           5
                 rooms per_household=test df["total rooms"] / test df["households"]
           6
           7
             train df = train df.assign(
           8
                 bedrooms per household=train_df["total_bedrooms"] / train_df["house
           9
          10
          11
             test_df = test_df.assign(
                 bedrooms per household=test df["total bedrooms"] / test df["household
          12
          13
          14
          15
             train df = train df.assign(
          16
                 population per household=train_df["population"] / train_df["househo
          17
          18
             test df = test df.assign(
          19
                 population per household=test_df["population"] / test_df["household
          20
```

In [14]: 1 train_df.head()

Out[14]:

	longitude	latitude	housing_median_age	total_rooms	total_bedrooms	population	households
6051	-117.75	34.04	22.0	2948.0	636.0	2600.0	602.0
20113	-119.57	37.94	17.0	346.0	130.0	51.0	20.0
14289	-117.13	32.74	46.0	3355.0	768.0	1457.0	708.0
13665	-117.31	34.02	18.0	1634.0	274.0	899.0	285.0
14471	-117.23	32.88	18.0	5566.0	1465.0	6303.0	1458.0

When is it OK to do things before splitting?

- Here it would have been OK to add new features before splitting because we are not using any global information about the feature values (e.g. the mean of a feature across rows), but only looking at one row at a time.
- But just to be safe and to avoid accidentally breaking the golden rule, it's better to do it after splitting.
- Question: Should we remove total_rooms , total_bedrooms , and population columns?
 - Probably. But I am keeping them in this lecture. You could experiment with removing them and examine whether results change.

Exploratory Data Analysis (EDA)

In [15]: 1 train_df.head()

Out[15]:

	longitude	latitude	housing_median_age	total_rooms	total_bedrooms	population	households
6051	-117.75	34.04	22.0	2948.0	636.0	2600.0	602.0
20113	-119.57	37.94	17.0	346.0	130.0	51.0	20.0
14289	-117.13	32.74	46.0	3355.0	768.0	1457.0	708.0
13665	-117.31	34.02	18.0	1634.0	274.0	899.0	285.0
14471	-117.23	32.88	18.0	5566.0	1465.0	6303.0	1458.0

The feature scales are quite different.

In [16]:

```
train_df.info()
```

<class 'pandas.core.frame.DataFrame'>
Int64Index: 18576 entries, 6051 to 19966
Data columns (total 13 columns):

Ducu	COTAMIND (COCAT 13 COTAMIND	, •		
#	Column	Non-Nu	ıll Count	Dtype
0	longitude	18576	non-null	float64
1	latitude	18576	non-null	float64
2	housing_median_age	18576	non-null	float64
3	total_rooms	18576	non-null	float64
4	total_bedrooms	18391	non-null	float64
5	population	18576	non-null	float64
6	households	18576	non-null	float64
7	median_income	18576	non-null	float64
8	median_house_value	18576	non-null	float64
9	ocean_proximity	18576	non-null	object
10	rooms_per_household	18576	non-null	float64
11	bedrooms_per_household	18391	non-null	float64
12	population_per_household	18576	non-null	float64
d+vne	es: float64(12), object(1)			

dtypes: float64(12), object(1)

memory usage: 2.0+ MB

We have one categorical feature and all other features are numeric features.

In [17]: 1 train_df.describe()

Out[17]:

	longitude	latitude	housing_median_age	total_rooms	total_bedrooms	populatio
count	18576.000000	18576.000000	18576.000000	18576.000000	18391.000000	18576.00000
mean	-119.565888	35.627966	28.622255	2635.749677	538.229786	1428.57816
std	1.999622	2.134658	12.588307	2181.789934	421.805266	1141.66480
min	-124.350000	32.540000	1.000000	2.000000	1.000000	3.00000
25%	-121.790000	33.930000	18.000000	1449.000000	296.000000	788.00000
50%	-118.490000	34.250000	29.000000	2127.000000	435.000000	1167.00000
75%	-118.010000	37.710000	37.000000	3145.000000	647.000000	1727.00000
max	-114.310000	41.950000	52.000000	39320.000000	6445.000000	35682.00000

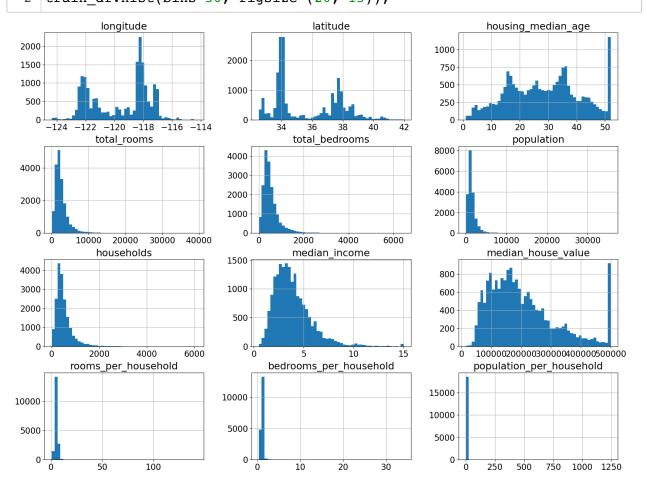
- Seems like total_bedrooms column has some missing values.
- This must have affected our new feature bedrooms_per_household as well.

```
In [18]: 1 housing_df["total_bedrooms"].isnull().sum()
```

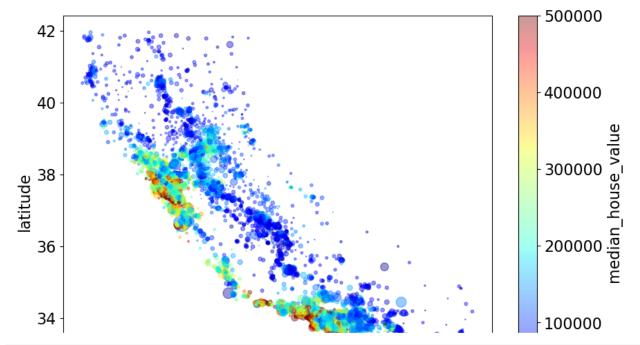
Out[18]: 207

In [19]:

1 ## (optional)
2 train df.hist(bins=50, figsize=(20, 15));



```
In [20]:
           1
              ## (optional)
              train df.plot(
           2
           3
                  kind="scatter",
           4
                  x="longitude",
                  y="latitude",
           5
           6
                  alpha=0.4,
           7
                  s=train_df["population"] / 100,
                  figsize=(10, 7),
           8
           9
                  c="median_house_value",
                  cmap=plt.get_cmap("jet"),
          10
          11
                  colorbar=True,
          12
                  sharex=False,
          13
              );
```



Was that all the transformations we need to apply to the dataset?

Here is what we see from the exploratory data analysis (EDA).

- Some missing values in total_bedrooms column.
- Scales are quite different across columns.
- Categorical variable ocean proximity.

Read about <u>preprocessing techniques implemented in scikit-learn (https://scikit-learn.org/stable/modules/preprocessing.html).</u>

Let's first run our baseline model DummyRegressor

```
In [22]:
              results dict = {} # dictionary to store our results for different mode
In [23]:
           1
              def mean std cross val scores(model, X train, y train, **kwargs):
           2
           3
                  Returns mean and std of cross validation
           4
           5
                  Parameters
           6
           7
                  model:
                      scikit-learn model
           8
           9
                  X train : numpy array or pandas DataFrame
          10
                      X in the training data
          11
                  y train:
          12
                      y in the training data
          13
          14
                  Returns
          15
                      pandas Series with mean scores from cross_validation
          16
          17
          18
                  scores = cross_validate(model, X_train, y_train, **kwargs)
          19
          20
          21
                  mean scores = pd.DataFrame(scores).mean()
          22
                  std scores = pd.DataFrame(scores).std()
          23
                  out col = []
          24
          25
                  for i in range(len(mean scores)):
                      out col.append((f"%0.3f (+/- %0.3f)" % (mean scores[i], std sco
          26
          27
                  return pd.Series(data=out col, index=mean scores.index)
          28
In [24]:
              dummy = DummyRegressor(strategy="median")
              results_dict["dummy"] = mean_std cross val scores(
           2
           3
                  dummy, X train, y train, return train score=True
           4
              )
In [25]:
           pd.DataFrame(results dict)
Out[25]:
                           dummy
                    0.002 (+/- 0.001)
             fit time
                    0.001 (+/- 0.000)
          score_time
           test_score -0.055 (+/- 0.012)
          train_score -0.055 (+/- 0.001)
```

Imputation

```
In [27]: 1 knn = KNeighborsRegressor()
2 knn.fit(X_train, y_train)
```

ValueError Traceback (most recent call las t) Cell In[27], line 2 1 knn = KNeighborsRegressor() ---> 2 knn.fit(X_train, y_train) File ~/miniconda3/envs/cpsc330/lib/python3.10/site-packages/sklearn/neigh bors/ regression.py:210, in KNeighborsRegressor.fit(self, X, y) 191 """Fit the k-nearest neighbors regressor from the training datase t. 192 193 Parameters 206 The fitted k-nearest neighbors regressor. 207 """ 208 self.weights = _check_weights(self.weights) --> 210 return self._fit(X, y) File ~/miniconda3/envs/cpsc330/lib/python3.10/site-packages/sklearn/neigh bors/_base.py:407, in NeighborsBase._fit(self, X, y) 405 if self. get tags()["requires y"]: if not isinstance(X, (KDTree, BallTree, NeighborsBase)): 406 --> 407 X, y = self._validate_data(X, y, accept_sparse="csr", multi_output=True, order 408 ="C" 409) 411 if is classifier(self): 412 # Classification targets require a specific format 413 **if** y.ndim == 1 **or** y.ndim == 2 **and** y.shape[1] == 1: File ~/miniconda3/envs/cpsc330/lib/python3.10/site-packages/sklearn/base. py:596, in BaseEstimator. validate data(self, X, y, reset, validate separ ately, **check params) y = check array(y, input name="y", **check y params) 594 595 else: --> 596 X, y = check X y(X, y, **check params)597 out = X, y599 if not no val X and check params.get("ensure 2d", True): File ~/miniconda3/envs/cpsc330/lib/python3.10/site-packages/sklearn/util s/validation.py:1074, in check_X_y(X, y, accept_sparse, accept_large_spar se, dtype, order, copy, force all finite, ensure 2d, allow nd, multi outp ut, ensure min samples, ensure min features, y numeric, estimator) estimator name = check estimator name(estimator) 1069 1070 raise ValueError(1071 f"{estimator name} requires y to be passed, but the targe t y is None" 1072 -> 1074 X = check array(1075 Χ, 1076 accept sparse=accept sparse, 1077 accept large sparse=accept large sparse, 1078 dtype=dtype, 1079 order=order, 1080 copy=copy,

```
1081
            force all finite=force all finite,
   1082
            ensure_2d=ensure_2d,
   1083
            allow nd=allow nd,
            ensure min samples=ensure min samples,
   1084
   1085
            ensure min features=ensure min features,
   1086
            estimator=estimator,
            input name="X",
   1087
   1088 )
   1090 y = check y(y, multi_output=multi_output, y_numeric=y_numeric, e
stimator=estimator)
   1092 check consistent length(X, y)
File ~/miniconda3/envs/cpsc330/lib/python3.10/site-packages/sklearn/util
s/validation.py:899, in check_array(array, accept_sparse, accept_large_sp
arse, dtype, order, copy, force all finite, ensure 2d, allow nd, ensure m
in_samples, ensure_min_features, estimator, input_name)
    893
                raise ValueError(
    894
                    "Found array with dim %d. %s expected <= 2."
    895
                    % (array.ndim, estimator_name)
    896
                )
            if force all finite:
    898
--> 899
                _assert_all_finite(
    900
                    array,
    901
                    input_name=input_name,
    902
                    estimator_name=estimator_name,
                    allow_nan=force_all_finite == "allow-nan",
    903
    904
                )
    906 if ensure min samples > 0:
            n samples = num samples(array)
File ~/miniconda3/envs/cpsc330/lib/python3.10/site-packages/sklearn/util
s/validation.py:146, in assert all finite(X, allow nan, msg dtype, estim
ator name, input name)
    124
                if (
    125
                    not allow nan
    126
                    and estimator name
   (\ldots)
    130
                    # Improve the error message on how to handle missing
values in
    131
                    # scikit-learn.
    132
                    msg err += (
                        f"\n{estimator_name} does not accept missing valu
    133
es"
    134
                         " encoded as NaN natively. For supervised learnin
q, you might want"
   (\ldots)
                         "#estimators-that-handle-nan-values"
    144
    145
                    )
                raise ValueError(msg err)
    148 # for object dtype data, we only check for NaNs (GH-13254)
    149 elif X.dtype == np.dtype("object") and not allow nan:
```

ValueError: Input X contains NaN.

KNeighborsRegressor does not accept missing values encoded as NaN nativel y. For supervised learning, you might want to consider sklearn.ensemble.H istGradientBoostingClassifier and Regressor which accept missing values e ncoded as NaNs natively. Alternatively, it is possible to preprocess the

data, for instance by using an imputer transformer in a pipeline or drop samples with missing values. See https://scikit-learn.org/stable/modules/impute.html (https://scikit-learn.org/stable/modules/impute.html) You can find a list of all estimators that handle NaN values at the following pag e: https://scikit-learn.org/stable/modules/impute.html#estimators-that-handle-nan-values (https://scikit-learn.org/stable/modules/impute.html#estimators-that-handle-nan-values)

What's the problem?

ValueError: Input contains NaN, infinity or a value too large for d type('float64').

- The classifier is not able to deal with missing values (NaNs).
- · What are possible ways to deal with the problem?
 - Delete the rows?
 - Replace them with some reasonable values?
- SimpleImputer is a transformer in sklearn to deal with this problem. For example:
 - You can impute missing values in categorical columns with the most frequent value.
 - You can impute the missing values in numeric columns with the mean or median of the column.

In [28]: 1 X_train.sort_values("bedrooms_per_household")

Out[28]:

	longitude	latitude	housing_median_age	total_rooms	total_bedrooms	population	households
20248	-119.23	34.25	28.0	26.0	3.0	29.0	9.0
12649	-121.47	38.51	52.0	20.0	4.0	74.0	9.0
3125	-117.76	35.22	4.0	18.0	3.0	8.0	6.0
12138	-117.22	33.87	16.0	56.0	7.0	39.0	14.0
8219	-118.21	33.79	33.0	32.0	18.0	96.0	36.0
•••							
4591	-118.28	34.06	42.0	2472.0	NaN	3795.0	1179.0
19485	-120.98	37.66	10.0	934.0	NaN	401.0	255.0
6962	-118.05	33.99	38.0	1619.0	NaN	886.0	357.0
14970	-117.01	32.74	31.0	3473.0	NaN	2098.0	677.0
7763	-118.10	33.91	36.0	726.0	NaN	490.0	130.0

18576 rows × 11 columns

```
In [29]: 1  X_train.shape
2  X_test.shape

Out[29]: (2064, 11)

In [32]: 1  imputer = SimpleImputer(strategy="median")
2  imputer.fit(X_train)
3  X_train_imp = imputer.transform(X_train)
4  X_test_imp = imputer.transform(X_test)
```

- · Let's check whether the NaN values have been replaced or not
- Note that imputer.transform returns an numpy array and not a dataframe

```
Out[37]: longitude
                                        0
          latitude
                                        0
          housing median age
                                        0
          total rooms
                                        0
          total bedrooms
                                        0
          population
                                        0
          households
                                        0
         median income
                                        0
          rooms per household
                                        0
          bedrooms per household
          population per household
                                        0
          dtype: int64
```

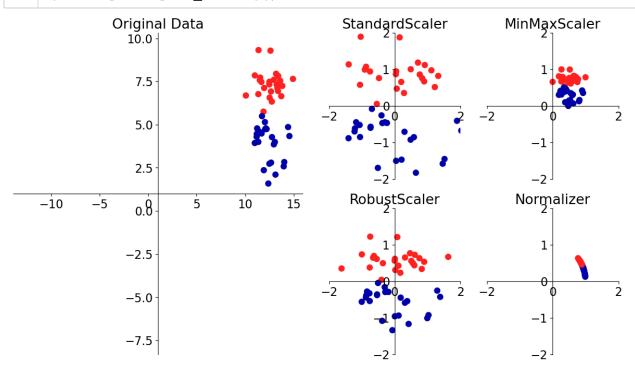
- Now the *k*-NN runs!
- The training error is bad though...

Out[38]: 0.5085407150708963

Scaling

- This problem affects a large number of ML methods.
- A number of approaches to this problem. We are going to look into the two most popular ones.

Approach	What it does	How to update X (but see below!)	
normalization	sets range to [0, 1]	<pre>X -= np.min(X,axis=0) X /= np.max(X,axis=0)</pre>	MinMaxScaler() (https://scikit-learn.org/stable/modul



In [40]: 1 from sklearn.preprocessing import MinMaxScaler, StandardScaler

Out[41]:

	longitude	latitude	housing_median_age	total_rooms	total_bedrooms	population	househo
0	0.908140	-0.743917	-0.526078	0.143120	0.235339	1.026092	0.2661
1	-0.002057	1.083123	-0.923283	-1.049510	-0.969959	-1.206672	-1.2533
2	1.218207	-1.352930	1.380504	0.329670	0.549764	0.024896	0.5428
3	1.128188	-0.753286	-0.843842	-0.459154	-0.626949	-0.463877	-0.5614
4	1.168196	-1.287344	-0.843842	1.343085	2.210026	4.269688	2.5009
18571	0.733102	-0.804818	0.586095	-0.875337	-0.243446	-0.822136	-0.9661
18572	1.163195	-1.057793	-1.161606	0.940194	0.609314	0.882438	0.7282
18573	-1.097293	0.797355	-1.876574	0.695434	0.433046	0.881563	0.5141
18574	-1.437367	1.008167	1.221622	-0.499947	-0.484029	-0.759944	-0.4544
18575	0.242996	0.272667	-0.684960	-0.332190	-0.353018	-0.164307	-0.3969

18576 rows × 11 columns

```
In [42]:
```

```
1 knn = KNeighborsRegressor()
```

- 2 knn.fit(X_train_scaled, y_train)
- 3 knn.score(X_train_scaled, y_train)

Out[42]: 0.8090877831586284

- Big difference in the KNN training performance after scaling the data.
- But we saw last week that training score doesn't tell us much. We should look at the cross-validation score.

? ? Questions for class discussion

True/False on scaling and imputation

- 1. StandardScaler ensures a fixed range (i.e., minimum and maximum values) for the features.
- 2. StandardScaler calculates mean and standard deviation for each feature separately.
- 3. In general, it's a good idea to apply scaling on numeric features before training k-NN or SVM RBF models.
- 4. After normalization, all numerical features in training and test set will have values between 0 and 1.
- 5. It is OK to modify features before splitting into training and testing set if the modification is row-wise.
 - 1. False
 - 2. True
 - 3. True
 - 4. False (not in the test set)
 - 5. True (but we don't recommend it)

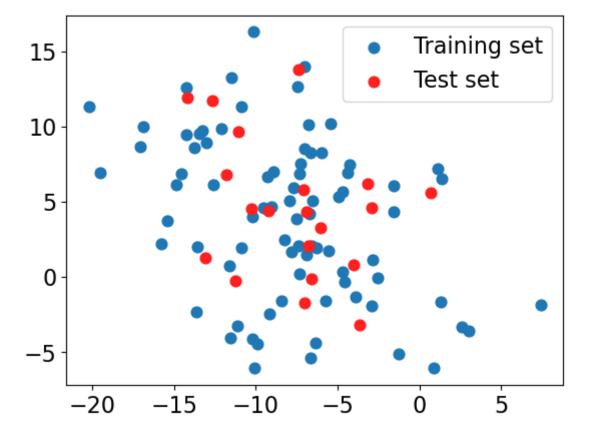
More True/False on scaling and imputation

- 4. The transformers such as StandardScaler or SimpleImputer in scikit-learn return a dataframe with transformed features.
- 5. The transformed feature values might be hard to interpret for humans.
- 6. After applying SimpleImputer, the transformed data has a different shape than the original data.

Consider a toy data with the following two columns. If you apply StandardScaler on this data, both columns A and B will end up being identical. True or False?

Let's create some synthetic data.

```
In [43]:
             from sklearn.datasets import make blobs, make classification
           2
           3
             # make synthetic data
           4
             X, y = make_blobs(n_samples=100, centers=3, random_state=12, cluster_st
             # split it into training and test sets
             X_train_toy, X_test_toy, y_train_toy, y_test_toy = train_test_split(
                 X, y, random_state=5, test_size=0.2
           8
             plt.scatter(X train_toy[:, 0], X train_toy[:, 1], label="Training set",
          9
          10
             plt.scatter(
                 X_test_toy[:, 0], X_test_toy[:, 1], color=mglearn.cm2(1), label="Te
          11
          12
             plt.legend(loc="upper right");
          13
```



Let's transform the data using StandardScaler and examine how the data looks like.

```
In [45]:
              plot original scaled(X train toy, X test toy, train transformed, test
                         Original Data
                                                               Properly transformed
           15
                                      Training set
                                                                                Training set
                                                     2
                                      Test set
                                                                                Test set
           10
                                                     1
            5
                                                     0
            0
                                                    -1
          -5
                                                    -2
              -20
                   -15
                                                          -2
In [46]:
             knn = KNeighborsClassifier()
              knn.fit(train_transformed, y_train_toy)
              print(f"Training score: {knn.score(train_transformed, y_train_toy):.2f}
              print(f"Test score: {knn.score(test_transformed, y_test_toy):.2f}")
          Training score: 0.75
          Test score: 0.55
```

Bad methodology 1: Scaling the data separately (for class discussion)

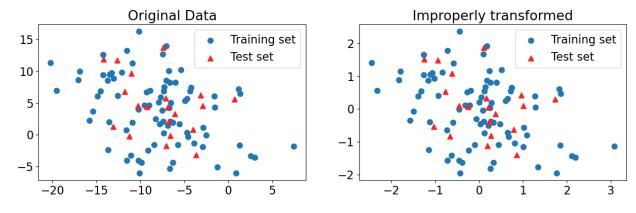
```
In [48]:
             # DO NOT DO THIS! For illustration purposes only.
          1
             scaler = StandardScaler()
             scaler.fit(X train toy)
             train scaled = scaler.transform(X train toy)
          5
             scaler = StandardScaler() # Creating a separate object for scaling tes
             scaler.fit(X test toy) # Calling fit on the test data
          7
             test scaled = scaler.transform(
          9
                 X test toy
             ) # Transforming the test data using the scaler fit on test data
          10
          11
          12
            knn = KNeighborsClassifier()
          13
             knn.fit(train scaled, y train toy)
             print(f"Training score: {knn.score(train scaled, y train toy):.2f}")
             print(f"Test score: {knn.score(test scaled, y test toy):.2f}")
```

Training score: 0.75
Test score: 0.50

• Is anything wrong in methodology 1? If yes, what is it?

```
In [49]:
           1
              plot_original_scaled(
           2
                  X train toy,
           3
                  X_test_toy,
           4
                  train_scaled,
           5
                  test scaled,
           6
                  title_transformed="Improperly transformed",
           7
                        Original Data
                                                             Improperly transformed
          15
                                     Training set
                                                                              Training set
                                                    2
                                      Test set
                                                                              Test set
          10
                                                    1
           5
                                                    0
           0
                                                   -1
          -5
                                                   -2
             -20
          Bad methodology 2: Scaling the data together (for class discussion)
In [51]:
          1 X train toy.shape, X test toy.shape
Out[51]: ((80, 2), (20, 2))
In [52]:
             # join the train and test sets back together
             XX = np.vstack((X_train_toy, X_test_toy))
             XX.shape
Out[52]: (100, 2)
In [53]:
             scaler = StandardScaler()
           1
           2 scaler.fit(XX)
           3 XX_scaled = scaler.transform(XX)
             XX_train = XX_scaled[:80]
           5 XX test = XX scaled[80:]
In [54]:
           1 knn = KNeighborsClassifier()
           2 knn.fit(XX train, y train toy)
             print(f"Training score: {knn.score(XX train, y train toy):.2f}") # Mis
              print(f"Test score: {knn.score(XX_test, y_test_toy):.2f}") # Misleadin
          Training score: 0.75
          Test score: 0.55
```

Is anything wrong in methodology 2? If yes, what is it?



Not a big difference in the transformed data but if the test set is large it might influence the mean and standard deviation significantly. **Importantly, this breaks the golden rule!**

Methodology 3: Cross validation with already preprocessed data (for class discussion)

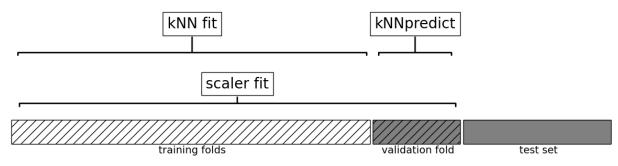
Out[56]:

	fit_time	score_time	test_score	train_score
0	0.000557	0.001731	0.6875	0.671875
1	0.000536	0.002388	0.7500	0.671875
2	0.000427	0.001202	0.6875	0.734375
3	0.000385	0.001151	0.6250	0.750000
4	0.000360	0.001179	0.5000	0.687500

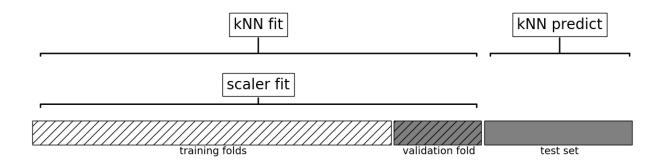
• Is there anything wrong in methodology 3? Are we breaking the golden rule here?

In [57]: 1 plot_improper_processing("kNN")

Cross validation



Test set prediction



In []: 1 plot_proper_processing("kNN")

Feature transformations and the golden rule [video ()]

How to carry out cross-validation?

- Last week we saw that cross validation is a better way to get a realistic assessment of the model.
- Let's try cross-validation with transformed data.

Out[58]:

	fit_time	score_time	test_score	train_score
0	0.012000	0.262788	0.710905	0.803734
1	0.008120	0.227898	0.706893	0.803212
2	0.008050	0.243732	0.711039	0.803030
3	0.008205	0.246907	0.695769	0.806275
4	0.007997	0.181020	0.697941	0.805146

- Do you see any problem here?
- Are we applying fit_transform on train portion and transform on validation portion in each fold?
 - Here you might be allowing information from the validation set to leak into the training step.
- You need to apply the **SAME** preprocessing steps to train/validation.
- With many different transformations and cross validation the code gets unwieldy very quickly.
- · Likely to make mistakes and "leak" information.
- In these examples our test accuracies look fine, but our methodology is flawed.
- Implications can be significant in practice!

Pipelines

Can we do this in a more elegant and organized way?

- YES!! Using <u>scikit-learn Pipeline (https://scikit-learn.org/stable/modules/generated/sklearn.pipeline.Pipeline.html)</u>.
- scikit-learn Pipeline (https://scikit-learn.org/stable/modules/generated/sklearn.pipeline.Pipeline.html) allows you to define a "pipeline" of transformers with a final estimator.

Let's combine the preprocessing and model with pipeline

```
In [59]:
             ### Simple example of a pipeline
             from sklearn.pipeline import Pipeline
           2
           3
           4
             pipe = Pipeline(
           5
                 steps=[
                      ("imputer", SimpleImputer(strategy="median")),
           6
           7
                      ("scaler", StandardScaler()),
                      ("regressor", KNeighborsRegressor()),
           8
           9
                  1
          10
             )
```

- · Syntax: pass in a list of steps.
- The last step should be a model/classifier/regressor.
- All the earlier steps should be **transformers**.

Alternative and more compact syntax: make pipeline

- Shorthand for Pipeline constructor
- · Does not permit naming steps
- Instead the names of steps are set to lowercase of their types automatically;
 StandardScaler() would be named as standardscaler

In a Jupyter environment, please rerun this cell to show the HTML representation or trust the notebook.

On GitHub, the HTML representation is unable to render, please try loading this page with nbviewer.org.

• Note that we are passing X train and **not** the imputed or scaled data here.

When you call fit on the pipeline, it carries out the following steps:

- Fit SimpleImputer on X train
- Transform X train using the fit SimpleImputer to create X_train_imp
- Fit StandardScaler on X_train_imp
- Transform X_train_imp using the fit StandardScaler to create
 X train imp scaled

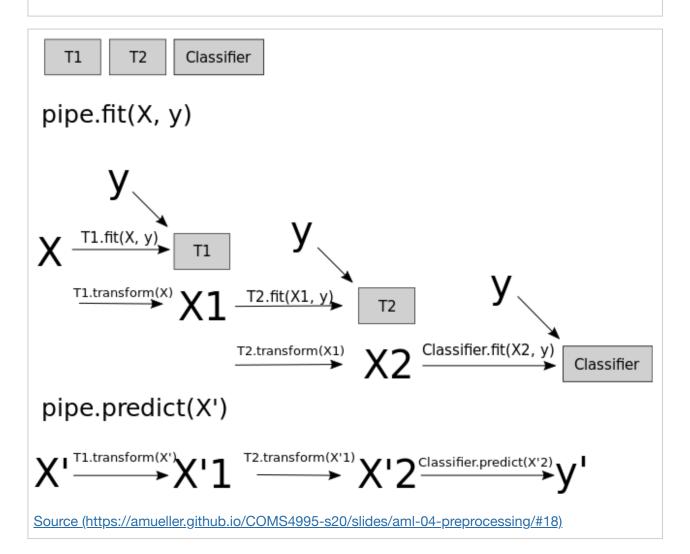
60420.])

• Fit the model (KNeighborsRegressor in our case) on X train imp scaled

```
In [62]:
          1 pipe.predict(X_train)
Out[62]: array([122460., 115220., 216940., ..., 240420., 254500.,
```

Note that we are passing original data to predict as well. This time the pipeline is carrying out following steps:

- Transform X_train using the fit SimpleImputer to create X_train_imp
- Transform X_train_imp using the fit StandardScaler to create X train imp scaled
- Predict using the fit model (KNeighborsRegressor in our case) on X train imp scaled.



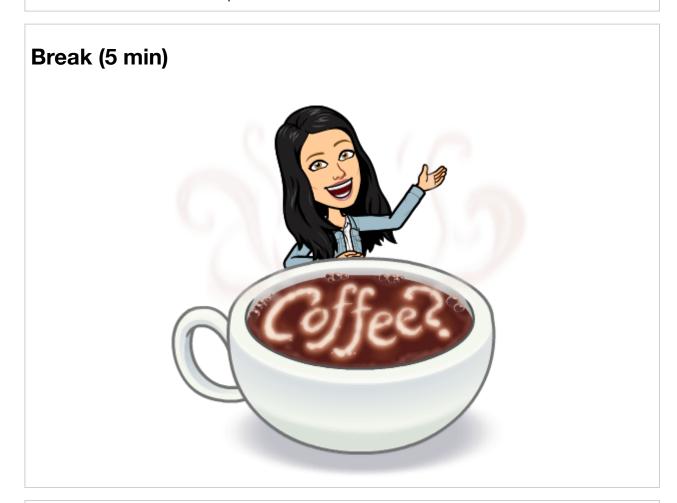
Let's try cross-validation with our pipeline

```
Out[63]:
```

```
        dummy
        0.002 (+/- 0.001)
        0.001 (+/- 0.000)
        -0.055 (+/- 0.012)
        -0.055 (+/- 0.001)

        imp + scaling + knn
        0.028 (+/- 0.003)
        0.254 (+/- 0.032)
        0.706 (+/- 0.006)
        0.806 (+/- 0.005)
```

Using a Pipeline takes care of applying the fit_transform on the train portion and only transform on the validation portion in each fold.



Categorical features [video (https://youtu.be/2mJ9rAhMMI0)]

- Recall that we had dropped the categorical feature ocean_proximity feature from the dataframe. But it could potentially be a useful feature in this task.
- Let's create our X_train and and X_test again by keeping the feature in the data.

```
In [64]: 1 test_df.head()
```

Out[64]:

	longitude	latitude	housing_median_age	total_rooms	total_bedrooms	population	households
19121	-122.64	38.24	40.0	1974.0	410.0	1039.0	398.0
20019	-119.05	36.09	9.0	3297.0	568.0	1749.0	568.0
15104	-116.98	32.85	12.0	3570.0	713.0	3321.0	666.0
3720	-118.42	34.20	27.0	3201.0	970.0	3403.0	948.0
8938	-118.47	34.01	41.0	2704.0	557.0	1047.0	478.0

• Let's try to build a KNeighborRegressor on this data using our pipeline

In [67]: 1 pipe.fit(X_train, X_train)

ValueError Traceback (most recent call las t) Cell In[67], line 1 ---> 1 pipe.fit(X_train, X_train) File ~/miniconda3/envs/cpsc330/lib/python3.10/site-packages/sklearn/pipel ine.py:378, in Pipeline.fit(self, X, y, **fit params) **352** """Fit the model. 353 354 Fit all the transformers one after the other and transform the 375 Pipeline with fitted steps. 376 """ 377 fit_params_steps = self._check_fit_params(**fit_params) --> 378 Xt = self. fit(X, y, **fit params steps) 379 with _print_elapsed_time("Pipeline", self._log_message(len(self.s teps) - 1)): if self. final estimator != "passthrough": 380 File ~/miniconda3/envs/cpsc330/lib/python3.10/site-packages/sklearn/pipel ine.py:336, in Pipeline. fit(self, X, y, **fit params steps) cloned_transformer = clone(transformer) 335 # Fit or load from cache the current transformer --> 336 X, fitted transformer = fit transform one cached(cloned transformer, 337 338 Х, 339 у, 340 None, message clsname="Pipeline", 341 342 message=self. log message(step idx), 343 **fit params steps[name], 344) 345 # Replace the transformer of the step with the fitted 346 # transformer. This is necessary when loading the transformer 347 # from the cache. 348 self.steps[step idx] = (name, fitted transformer) File ~/miniconda3/envs/cpsc330/lib/python3.10/site-packages/joblib/memor y.py:349, in NotMemorizedFunc. call (self, *args, **kwargs) 348 def call (self, *args, **kwargs): --> 349 return self.func(*args, **kwargs) File ~/miniconda3/envs/cpsc330/lib/python3.10/site-packages/sklearn/pipel ine.py:870, in fit transform one(transformer, X, y, weight, message clsn ame, message, **fit params) 868 with _print_elapsed_time(message clsname, message): if hasattr(transformer, "fit transform"): 869 --> 870 res = transformer.fit transform(X, y, **fit params) 871 else: 872 res = transformer.fit(X, y, **fit params).transform(X) File ~/miniconda3/envs/cpsc330/lib/python3.10/site-packages/sklearn/base. py:870, in TransformerMixin.fit_transform(self, X, y, **fit_params) return self.fit(X, **fit params).transform(X) 867 868 else:

```
# fit method of arity 2 (supervised transformation)
    869
--> 870
            return self.fit(X, y, **fit_params).transform(X)
File ~/miniconda3/envs/cpsc330/lib/python3.10/site-packages/sklearn/imput
e/ base.py:364, in SimpleImputer.fit(self, X, y)
    355 if self.verbose != "deprecated":
    356
           warnings.warn(
                "The 'verbose' parameter was deprecated in version "
    357
    358
                "1.1 and will be removed in 1.3. A warning will "
   (\ldots)
    361
                FutureWarning,
    362
            )
--> 364 X = self. validate input(X, in fit=True)
    366 # default fill value is 0 for numerical input and "missing value"
    367 # otherwise
    368 if self.fill_value is None:
File ~/miniconda3/envs/cpsc330/lib/python3.10/site-packages/sklearn/imput
e/ base.py:317, in SimpleImputer. validate input(self, X, in fit)
    311 if "could not convert" in str(ve):
    312
            new ve = ValueError(
    313
                "Cannot use {} strategy with non-numeric data:\n{}".forma
t(
    314
                    self.strategy, ve
    315
                )
    316
            raise new_ve from None
--> 317
    318 else:
    319
           raise ve
```

ValueError: Cannot use median strategy with non-numeric data:
could not convert string to float: 'INLAND'

- This failed because we have non-numeric data.
- Imagine how k-NN would calculate distances when you have non-numeric features.

Can we use this feature in the model?

- In scikit-learn, most algorithms require numeric inputs.
- Decision trees could theoretically work with categorical features.
 - However, the sklearn implementation does not support this.

What are the options?

- Drop the column (not recommended)
 - If you know that the column is not relevant to the target in any way you may drop it.
- We can transform categorical features to numeric ones so that we can use them in the model.
 - Ordinal encoding (https://scikitlearn.org/stable/modules/generated/sklearn.preprocessing.OrdinalEncoder.html) (occasionally recommended)

One-hot encoding (recommended in most cases) (this lecture)

```
In [68]:
            1
               X_toy = pd.DataFrame(
            2
                    {
            3
                        "language": [
            4
                             "English",
            5
                             "Vietnamese",
                             "English",
            6
            7
                             "Mandarin",
            8
                             "English",
                             "English",
            9
           10
                             "Mandarin",
           11
                             "English",
                             "Vietnamese",
           12
                             "Mandarin",
           13
           14
                             "French",
                             "Spanish",
           15
           16
                             "Mandarin",
                             "Hindi",
           17
           18
                        ]
           19
                    }
           20
           21
               X_toy
```

Out[68]:

language

- 0 English
- 1 Vietnamese
- 2 English
- 3 Mandarin
- 4 English
- 5 English
- 6 Mandarin
- **7** English
- 8 Vietnamese
- 9 Mandarin
- 10 French
- 11 Spanish
- 12 Mandarin
- 13 Hindi

Ordinal encoding (occasionally recommended)

- Here we simply assign an integer to each of our unique categorical labels.
- We can use sklearn's <u>OrdinalEncoder (https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.OrdinalEncoder.html)</u>.

Out[69]:

	language	language_enc
0	English	0.0
1	Vietnamese	5.0
2	English	0.0
3	Mandarin	3.0
4	English	0.0
5	English	0.0
6	Mandarin	3.0
7	English	0.0
8	Vietnamese	5.0
9	Mandarin	3.0
10	French	1.0
11	Spanish	4.0
12	Mandarin	3.0
13	Hindi	2.0

What's the problem with this approach?

- We have imposed ordinality on the categorical data.
- For example, imagine when you are calculating distances. Is it fair to say that French and Hindi are closer than French and Spanish?
- In general, label encoding is useful if there is ordinality in your data and capturing it is important for your problem, e.g., [cold, warm, hot].

One-hot encoding (OHE)

- Create new binary columns to represent our categories.
- If we have *c* categories in our column.
 - We create c new binary columns to represent those categories.
- Example: Imagine a language column which has the information on whether you
- We can use sklearn's <u>OneHotEncoder (https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.OneHotEncoder.html)</u> to do so.

One-hot encoding is called one-hot because only one of the newly created features is 1 for each data point.

```
In [70]:
             from sklearn.preprocessing import OneHotEncoder
           1
           2
           3
             enc = OneHotEncoder(handle_unknown="ignore", sparse=False)
             enc.fit(X_toy)
             X toy ohe = enc.transform(X toy)
             pd.DataFrame(
           7
                 data=X toy ohe,
           8
                 columns=enc.get_feature_names_out(["language"]),
                  index=X toy.index,
           9
          10
```

Out[70]: language_English language_French language_Hindi language_Mandarin language_Spanish langu 0 1.0 0.0 0.0 0.0 0.0 1 0.0 0.0 0.0 0.0 0.0 2 1.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 3 1.0 1.0 0.0 0.0 0.0 0.0 4 5 1.0 0.0 0.0 0.0 0.0 0.0 0.0 6 0.0 1.0 0.0 0.0 0.0 0.0 0.0 7 1.0 8 0.0 0.0 0.0 0.0 0.0 9 0.0 0.0 0.0 1.0 0.0 10 0.0 1.0 0.0 0.0 0.0 11 0.0 0.0 0.0 0.0 1.0 12 0.0 0.0 0.0 1.0 0.0

1.0

0.0

Let's do it on our housing data

0.0

13

• We can look at the new features created using categories attribute

0.0

0.0

Out[73]:

	ocean_proximity_<1H OCEAN	ocean_proximity_INLAND	ocean_proximity_ISLAND	ocean_proximity_NE# B#
6051	0	1	0	
20113	0	1	0	
14289	0	0	0	
13665	0	1	0	
14471	0	0	0	
7763	1	0	0	
15377	1	0	0	
17730	1	0	0	
15725	0	0	0	
19966	0	1	0	

18576 rows × 5 columns

One-hot encoded variables are also referred to as **dummy variables**. You will often see people using <u>get dummies method of pandas</u>

(https://pandas.pydata.org/docs/reference/api/pandas.get dummies.html) to convert categorical variables into dummy variables. That said, using sklearn 's OneHotEncoder has the advantage of making it easy to treat training and test set in a consistent way.

? ? Questions for class discussion

True/False: Pipelines and one-hot encoding

1. You can "glue" together imputation and scaling of numeric features and scikit-learn classifier object within a single pipeline.

- 2. You can "glue" together scaling of numeric features, one-hot encoding of categorical features, and scikit-learn classifier object within a single pipeline.
- 3. Pipelines will fit and transform on the training fold and only transform on the validation fold during cross-validation.
- 4. What's the better encoding for weather labels such as "sunny". "overcast" and "rainy"?
 - 1. True
 - 2. Not yet (we'll find a way)
 - 3. True
 - 4. One-hot

What did we learn today?

- Motivation for preprocessing
- · Common preprocessing steps
 - Imputation
 - Scaling
 - One-hot encoding
- · Golden rule in the context of preprocessing
- Building simple supervised machine learning pipelines using sklearn.pipeline.make_pipeline.

Problem: Different transformations on different columns

- · How do we put this together with other columns in the data before fitting the regressor?
- · Before we fit our regressor, we want to apply different transformations on different columns
 - Numeric columns
 - imputation
 - scaling
 - Categorical columns
 - imputation
 - one-hot encoding

Coming up: sklearn's ColumnTransformer (https://scikit-

<u>learn.org/stable/modules/generated/sklearn.compose.ColumnTransformer.html)</u>!!

In []:

1